Gap inhomogeneities and the density of states in disordered d-wave superconductors

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We report on a numerical study of disorder effects in 2D d-wave BCS superconductors. We compare exact numerical solutions of the Bogoliubov-deGennes (BdG) equations for the density of states $\rho(E)$ with the standard T-matrix approximation. Local suppression of the order parameter near impurity sites, which occurs in self-consistent solutions of the BdG equations, leads to apparent power law behavior $\rho(E) \sim |E|^{\alpha}$ with non-universal α over an energy scale comparable to the single impurity resonance energy Ω_0. We show that the novel effects arise from static spatial correlations between the order parameter and the impurity distribution.

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In spite of strong electronic correlations in the normal state, the superconducting state of high T_c materials seems to be accurately described by a conventional BCS-like phenomenology. The debate over the k-space structure of the BCS order parameter $\Delta_{\mathbf{k}}$ has now been resolved in favour of pairing states with d-wave symmetry. Since this symmmetry implies that $\Delta_{\mathbf{k}}$ changes sign under rotation by $\pi/2$, there are necessarily points on the 2D Fermi surface at which $\Delta_{\mathbf{k}}$ vanishes. The unique low-energy properties of high T_c superconductors are determined by the quasiparticle excitations in the vicinity of these nodal points.

For conventional s-wave superconductors, the density of states (DOS) $\rho(E)$ has a well defined gap and is largely unaffected by non-magnetic disorder. In contrast, $\rho(E) \propto |E|$ in clean d-wave superconductors, and can be substantially altered by disorder. Much of the current understanding of disorder effects comes from perturbative theories, such as the widely-used self-consistent T-matrix approximation (SCTMA). In particular, the SCTMA is exact in the limit of a single impurity, and has been used in studies of the local DOS near an isolated scatterer [1]. For sufficiently strong scatterers, an isolated impurity introduces a pair of resonances at energies $\pm\Omega_0$ [2,3], where $\Omega_0 < \Delta$ is a function of of the impurity potential u_0 and of the band asymmetry. Analytic expressions for $\Omega_0(u_0)$ have been given for a symmetric band [2], and in this special instance the unitary limit $\Omega_0 \to 0$ coincides with $u_0 \to \infty$. For a realistic (asymmetric) band, the relationship is more complex [3].

For a finite concentration of impurities n_i, the SCTMA predicts that the impurity resonances broaden, with tails which overlap at the Fermi energy, leading to a finite residual DOS $\rho(0)$ [3–8]. The region over which $\rho(E) \approx \rho(0)$, the "impurity band", and has a width comparable to the scattering rate γ at $E = 0$. In the Born limit, the $\pm\Omega_0$ resonances are widely separated in energy, and the overlap of their tails is exponentially small. In the strong-scattering limit, however, the overlap is substantial and $\gamma \sim \sqrt{\Gamma\Delta_d}$, where Δ_d is the magnitude of the d-wave gap, $\Gamma = n_i/\pi N_0$ is the scattering rate in the normal state, and N_0 is the 2D normal-state DOS at the Fermi level. Several recent experiments [9–12] have studied quasiparticles in the impurity band in Zn-doped high T_c materials. Of particular note are attempts to verify a provocative prediction [10,11] that transport coefficients on energy scales ω, $T < \gamma$ have a universal value, independent of Γ [13,14].

The SCTMA which forms the basis of this world-view has several limitations. It is an effective medium theory, in which one solves for the eigenstates of an isolated impurity in the presence of a homogeneous mean-field representing all other impurities. This approach ignores multiple impurity scattering processes which are responsible for localization physics in metals and may lead to novel effects in 2D d-wave superconductors [13,15,16]. Another limitation of most SCTMA calculations is the use of a δ-function potential as an impurity model. While this simplifies the calculation substantially, numerical results hint that the detailed structure of the impurity potential may be important [8]. A related issue, which will be discussed at length in this Letter, is inhomogeneous order-parameter suppression. It is well-known that d-wave superconductivity is destroyed locally near a strong scatterer, and in the single-impurity limit [19,20], the additional scattering was found to renormalise Ω_0 but, surprisingly, to leave most other details of the scattered eigenstates unchanged. Here we show, using exact numerical solutions of the Bogoliubov-deGennes (BdG) equations, that additional novel physics *does* arise in the many-impurity case.

The main results of this work are summarised in Fig. 1. For a homogeneous order parameter, $\rho(E)$ saturates at a constant value as $E \to 0$ (in agreement with SCTMA), down to a mesoscopic energy scale $\sim 1/\rho L^2$ where level repulsion across the Fermi surface induces a gap. This small gap may be a precursor to a regime associated with strong localization in the thermodynamic limit as discussed by Senthil et al. [16]. These authors predicted asymptotic power-law behavior in $\rho(E)$ over an exponentially small energy scale $E_2 \sim 1/\rho(0)\xi_L^2$, where $\rho(0)$ is the residual density of states in the impurity band plateau

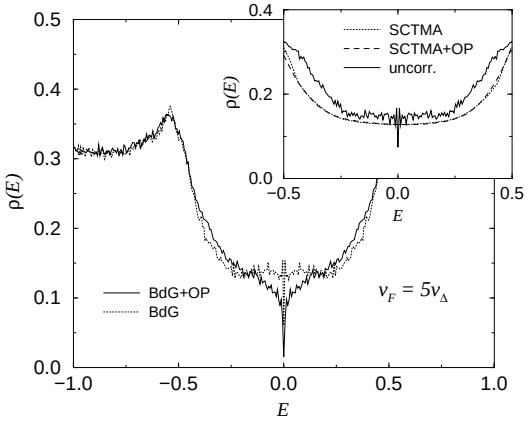

FIG. 1. Density of states for $n_i = 0.04$ and $u_0 = 10$. Numerical solutions of the BdG equations are shown with (BdG+OP) and without (BdG) self-consistent calculation of Δ_{ij}. Inset: T-matrix calculations of $\rho(E)$ with (SCTMA+OP) and without (SCTMA) off-diagonal scattering. Also shown is a model with uncorrelated impurity and off-diagonal potentials (uncorr.).

and $\xi_L \sim (v_F/\gamma)\exp(v_F/v_\Delta + v_\Delta/v_F)$ is the quasiparticle localization length. (v_F is the Fermi velocity and v_Δ is the gradient of Δ_k along the Fermi surface at the gap node). The actual value of the DOS at $E = 0$ is consistent with zero but not determined in our work; theoretically this point is still controversial. [18]

Figure 1 shows that when the order parameter is determined *self-consistently* from the BdG equations $\rho(E)$ is quite different. At low energies the DOS can be fit to a power law $\rho(E) \sim |E|^\alpha$ with nonuniversal α (Fig. 2). The power-law is the result of spatial correlations between the order-parameter and the impurity potential, and is therefore fundamentally different from those of Nersesyan *et al.* [15] and Senthil *et al* [16], where asymptotic power-laws were found, with $\alpha = 1/7$ and $\alpha = 1$ respectively. Unlike the DOS, the dimensionless conductance and inverse participation ratio (Fig. 3) are not changed significantly by self-consistency. Finally, we remark that the energy scale for the low-energy regime is $\gtrsim \Omega_0$, which is orders of magnitude larger than E_2 for realistic parameters.

We employ a one-band lattice model with nearest neighbour hopping amplitude t and a nearest neighbour attractive interaction V. Substitutional impurities are represented by a change in the on-site atomic energy. The Hamiltonian is

$$\mathcal{H} = -t\sum_{\langle i,j\rangle}\sum_{\sigma} c^\dagger_{i\sigma}c_{j\sigma} - \sum_{i,\sigma}[\mu - U_i]c^\dagger_{i\sigma}c_{i\sigma} - \sum_{\langle i,j\rangle}\{\Delta_{ij}c^\dagger_{i\uparrow}c^\dagger_{j\downarrow} + h.c.\}, \quad (1)$$

where the angle-brackets indicate that site indices i and j are nearest neighbours, U_i is the impurity potential which takes the value u_0 at a fraction n_i of the sites and is zero elsewhere, and $\Delta_{ij} = -V\langle c_{j\downarrow}c_{i\uparrow}\rangle$ is the mean-field order parameter, determined self-consistently by diagonalizing Eq. (1). Throughout this work, energies are measured in units of t, where t is of order 100 meV for high T_c materials. In non-self-consistent calculations the OP has the familiar k-space form $\Delta_k = \Delta_d[\cos(k_x) - \cos(k_y)]$, where $\Delta_d = \frac{1}{2}\sum_\pm(\Delta_{i\,i\pm x} - \Delta_{i\,i\pm y})$ is independent of i. Unless otherwise stated, $V = -2.3$ and $\mu = 1.2$ which yields $\Delta_d = 0.4$ (corresponding to $v_F/v_\Delta \approx 5$) in the absence of disorder. Self-consistent solutions show that Δ_{ij} is suppressed within a few lattice constants of each strongly-scattering impurity. Throughout this Letter, curves marked BdG and BdG+OP refer to the neglect or inclusion of self-consistency in Δ_{ij}.

The DOS is $\rho(E) = L^{-2}\sum_\alpha \delta(E - E_\alpha)$, where L is the linear system size and E_α are the discrete eigenenergies of $\mathcal{H}$. Our numerical calculations were performed on periodically continued systems with $L \le 45$. Typical DOS curves were obtained for $L = 25$ by averaging $\rho(E)$ over $\sim 50 - 500$ impurity configurations and $\sim 50 - 100$ k-vectors in the supercell Brillouin-zone. For system sizes $L \ge 35$, computational constraints restricted us to real periodic and anti-periodic boundary conditions.

An important motivation for the present study is the need for a test of the reliability of SCTMA predictions. Thus, we use the same disordered lattice model for the SCTMA as for the BdG calculations. We would also like to model order-parameter suppression within a self-consistent T-matrix approximation (SCTMA+OP), [17] and follow the ansatz of [19] that the off-diagonal potential is $\delta\Delta_{ij} = -\Delta_{ij}[\delta_{i,0} + \delta_{j,0}]$. This term appears in the off-diagonal block of the effective potential. In both cases, the T-matrix is a 2×2 matrix in particle-hole space which satisfies

$$T_{ij}(E) = U_{ij} + \sum_{R,R'} U_{iR}G(R - R', E)T_{R'j}(E), \quad (2a)$$

where G has the Fourier transform,

$$G_k(E) = \left[E\tau_0 - \epsilon_k\tau_3 - \Delta_k\tau_1 - \Sigma_k(E)\right]^{-1}, \quad (2b)$$

ϵ_k is the tight-binding dispersion, τ_i are the Pauli matrices, and $\Sigma_k(E) = n_iT_{kk}(E)$. Equation (2a) is solved in real-space to take advantage of the short range of the effective potential U. Finally, $\rho(E) = -\pi^{-1}L^{-2}\mathrm{Im}\sum_k \mathrm{Tr}\, G_k(E)$, where the trace is over particle-hole indices.

Except for the mesoscopic gap discussed previously, the BdG curve in Fig. 1 is quantitatively similar to the SCTMA (inset). In contrast, the BdG+OP curve vanishes smoothly as $E \to 0$, indicating that qualitatively new physics has been introduced by the inclusion of order parameter suppression. To emphasize that this result is unexpected, we point to the popular "Swiss cheese" model, in which it is assumed that pair-breaking causes a pocket of normal metal of radius ξ_0 (the coherence

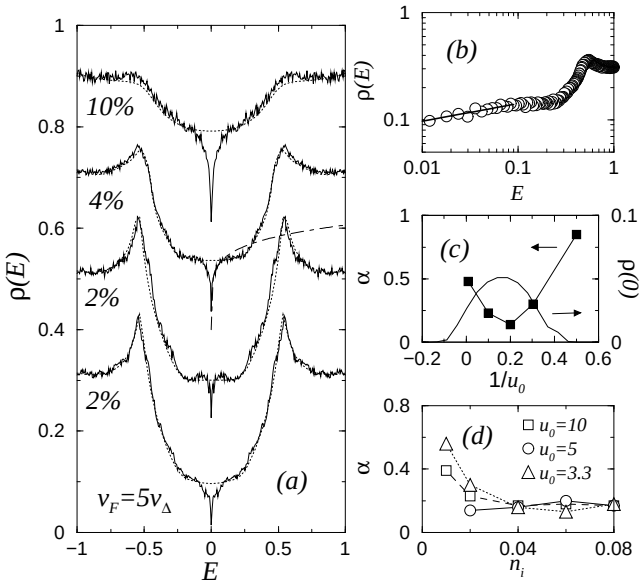

FIG. 2. Dependence of $\rho(E)$ on n_i and u_0: (a) BdG+OP (solid) and SCTMA (dotted) for $u_0 = 5$ (top three curves) and $u_0 = 10$ (bottom). Also shown (dot-dash) is a fit $\rho(E) = A|E|^\alpha$ for $n_i = 0.04$. (b) Logarithmic plot showing power law behavior for $n_i = 0.04$, $u_0 = 5$. (c) Dependence of power law on u_0 for $n_i = 0.02$. For comparison, SCTMA of $\rho(0)$ vs. u_0 is shown. Unitary limit is $u_0 \approx 5$. (d) Scaling of power law with n_i. Note that when $n_i = 0$, $\alpha = 1$.

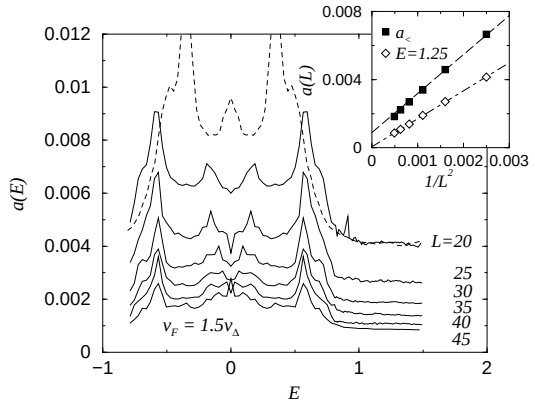

FIG. 3. Scaling of the inverse participation ratio for BdG+OP (solid curves) calculations. A BdG calculation (dashed) is also shown for $L = 20$. Parameters are $V = -4.47$ ($\Delta_d = 1.34$), $n_i = 0.06$, and $\mu = 1.0$ with between 14 (L=45) and 500 (L=20) impurity configurations and real boundary-conditions. Inset: Scaling inside and outside the impurity band. $a_<$ is the average of $a(E)$ for $|E| < 0.8$.

length) to form around each impurity. Within this model, $\rho(0)$ is *enhanced* relative to the SCTMA by $\sim n_i N_0 \xi_0^2$.

We emphasize that the correct spatial correlations between an impurity configuration and its self-consistent off-diagonal potentials must be preserved for the BdG+OP results to arise. This point is illustrated with a simple numerical calculation (inset of Fig. 1), in which Δ_{ij} is found self-consistently for random impurity distributions which are different from those appearing in the diagonal block of $\mathcal{H}$. The system therefore has two distinct types of impurity, one of which is purely off-diagonal, with uncorrelated distributions. It is striking that there is no hint of the correct low-energy behaviour in this calculation.

It is instructive to compare the BdG+OP result with the SCTMA+OP (inset, Fig. 1), since they include off-diagonal scattering from the order parameter at different levels of approximation. Furthermore, the SCTMA+OP does preserve the correlation between impurity location and order-parameter suppression. It has been used succesfully to describe shifts in Ω_0 due to off-diagonal scattering [19,20] but, here, fails to reproduce the correct low energy DOS in the bulk disordered case. Instead, $\rho(E)$ is quantitatively similar to the SCTMA, which is a direct result of the relative smallness of the off-diagonal potential $\Delta_d/u_0 \approx 0.04$.

In Fig. 2 we illustrate the dependence of the low energy DOS on both n_i and u_0. In Fig. 2(a) a series of curves shows how the low-energy regime scales towards zero-width as $n_i \to 0$ for the near-unitary scattering potential $u_0 = 5$ [21]. That the size of the regime should scale faster than γ with n_i is consistent with our earlier assertion that the novel behavior stems from a multiple-impurity effect. The details of the dilute impurity limit depend on the particular value of u_0 however: at 2% impurity concentration, the low-energy regime is significantly larger for $u_0 = 10$, which lies farther from unitarity, than for $u_0 = 5$. For fixed n_i, we find that the low-energy regime is $\gtrsim \Omega_0$.

In Fig. 2(b), a logarithmic plot of $\rho(E)$ reveals that the low energy DOS has an apparent power-law dependence on E, with non-universal exponent $0 < \alpha < 1$ [Fig. 2(c),(d)]. At low impurity concentrations, α is a strong function of both n_i and u_0, with α a minimum for unitary scatterers. For larger n_i, α appears to saturate at a value which is independent of u_0. We assert that this power law is fundamentally different from those reported elsewhere [15,16], since it is only observed when off-diagonal scattering is present and, as we will see next, is unrelated to strong quasiparticle localization.

We have studied the scaling of both the inverse participation ratio $a(E)$ and the Thouless number $g(E)$ with system size. The inverse participation ratio is defined in the usual way, $a(E) = x_4(E)/x_2(E)^2$, where $x_m(E) = [\rho(E)L^2]^{-1} \sum_{n,r} [|u_n(r)|^m + |v_n(r)|^m] \delta(E - E_n)$ and $u_n(r)$ and $v_n(r)$ are the particle and hole eigenfunctions, and is plotted in Fig. 3 for several system sizes. $a(E)$ is a direct measure of the spatial extent of the wavefunction; it scales as $1/L^2$ for extended states and is constant for states with localization length $\xi_L < L$.

The scaling and energy dependence of $a(E)$ is in general agreement with ref. [22] where calculations were made with similar parameters—there is a crossover in scaling between $E < \gamma$ and $E > \gamma$ consistent with a shorter localization length in the impurity band. Unlike ref. [22], we do not find saturation in $a_<$ [the average of $a(E < \gamma)$] for $L \leq 45$. For larger disorder concentrations (not shown) where $\xi_L < 45$ sites, we find that $a(E)$ saturates at $E = 0$ first indicating that $\xi_L(E)$ is an increasing function of E in the impurity band. The most important result for this work is that $a(E)$, and therefore ξ_L, is not significantly different in the BdG and BdG+OP calculations despite a substantial difference in $\rho(E)$. In the calculation which is shown, $a(E)$ is actually *decreased* slightly by self-consistency, corresponding to a slight *increase* in the localisation length.

We have also studied the Thouless number, defined as $g(E) = \sum_n [E_n(\pi) - E_n(0)]\delta(E - E_n)$, where the argument of E_n refers to the application of periodic or antiperiodic boundary conditions in the x-direction. As L is increased, $g(E)$ is expected to cross over from a constant in the diffusive regime to exponential scaling indicative of strong localization. For $L \leq 45$ we find no significant scaling of $g(E)$ with L, consistent with what is found for $a(E)$. Most significantly, we find that $g(E)$ is nearly identical in the BdG and BdG+OP calculations, even for low-energy states where substantial changes in $\rho(E)$ occur.

This behaviour is reminiscent of what is seen in Hartree-Fock studies of interacting electrons in disordered conductors [24]. There, the Coulomb interaction enforces spatial correlations between the disorder and charge distributions and leads to the formation of a gap in $\rho(E)$ [23], yet leaves the dimensionless conductance (a two-particle property related to the Thouless number) unchanged. The power-law DOS we observe here may have a similar origin; it is certainly clear that $\rho(E)$ depends crucially on the spatial correlations between the impurity potential and d-wave order parameter. In the current work, however, it is the pairing interaction which is relevant and the BdG equations provide a mean-field description of the pairing interaction which is analogous to the Hartree-Fock description of the Coulomb interaction. We speculate that the short-ranged pairing interaction produces spatial correlations between distant impurities via the overlap of the long range tails [2] of the single impurity resonances.

In this work we have shown that spatial correlations between order parameter and impurity distributions in d-wave superconductors lead to apparent power-laws in $\rho(E)$ at low energies. These results are potentially relevant to quasi-2D superconductors like BSCCO-2212. Unfortunately, most disorder studies have been performed on the anisotropic 3D YBCO system, where correlation effects are expected to be less pronounced. Indeed there is considerable evidence, particularly in Zn-substituted YBCO, that disorder does indeed induce a finite DOS at the Fermi level [9,10,12] and somewhat weaker evidence that it scales with disorder in accordance with the SCTMA [9]. Our work should therefore provide a strong motivation to study Zn doping, and other types of planar disorder, in the quasi-2D BSCCO-2212 system at low temperatures.

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